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APPARATUS AND METHOD FOR THE MEASUREMENT OF DIFFRACTING STRUCTURES

James M. Holden
William A. McGahan
Richard A. Yarussi
Pablo I. Rovira
Roger R. Lowe-Webb

FIELD OF THE INVENTION

This invention relates in general to metrology devices and in particular to metrology devices that may be used to measure diffracting structures.

BACKGROUND

It is desirable to measure circuit structures and other types of structures, e.g., resist structures, during the production of integrated circuits. Optical metrology tools are particularly well suited for measuring microelectronic structures because they are nondestructive, accurate, repeatable, fast, and inexpensive. Often different metrology tools are required to measure different structures or parameters on a wafer. For example, certain structures on a wafer act as diffraction gratings, which conventionally require a different metrology tool, e. g. critical dimension-scanning electron microscopy (CD-SEM), than is used to measure planar thin films.

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One tool that is sometimes used to measure diffracting structures is a scatterometer. Scatterometry is an angle-resolved measurement and characterization of light scattered from a structure. Scatterometry is discussed in detail in U.S. Serial No. 09/036,557, filed March 6, 1998, which is assigned to KLA-Tencor Corporation, which has an International Publication No. WO 99/45340, dated September 10, 1999, and which is incorporated herein by reference.

U.S. Serial No. 09/036,557 discloses the use of a spectroscopic ellipsometer to measure the diffracting structure. The sampling beam is incident on the sample at an oblique angle. The incident light of the spectroscopic ellipsometer is polarized to provide a beam in the TE mode (S-polarized) when the incidence plane of the beam is perpendicular to the grating of the diffracting structure or to provide a beam in the TM mode (P-polarized) when the incidence plane of the beam is parallel to the grating. Aligning the incident radiation with the grating of the diffracting

structure unfortunately is difficult, particularly where the wafer stage is an r-θ stage. With an r-θ stage, the entire metrology apparatus must be rotated to properly align the incident radiation with the grating. U.S. Serial No. 09/036,557 discloses a dedicated scatterometer instrument that uses a spectroscopic ellipsometer with non-normal incident light and that is used in a scatterometer mode.

In addition, U.S Serial No. 09/036,557 teaches that a reference database is generated using optical modeling. The reference database is simplified by measuring the film thickness and optical indices of film underlying the diffracting structure. Thus, prior to ellipsometrically measuring the diffraction grating, a measurement of the underlying film is performed. A broadband ellipsometric measurement is then made at a single polarization orientation, and the reference database is consulted to determine the structure of the diffraction grating. As can be seen, even though the size of the database is reduced by measuring the film thickness and optical indices of the underlying film, this process still requires the generation of a relatively large database. Further, the sample or metrology device must be moved and refocused to measure the underlying film, i.e., without the diffracting structure, and the diffracting structure itself, which is time intensive.

Thus, what is needed is an optical metrology tool to quickly and accurately measure diffraction gratings, as well as other non-diffracting structures, and that may be used with various wafer stages, including X,Y,Z, θ stages, as well as stages capable of r-θ movement only.

SUMMARY

A normal incidence reflectometer uses normally incident broadband radiation to measure one or more parameters of a diffracting structure. A rotatable analyzer/polarizer is used to analyze the diffracted radiation that is reflected off the diffracting structure. Relative rotation of the rotatable analyzer/polarizer with respect to the diffracting structure permits analysis of the diffracted radiation at multiple polarity orientations. The analyzer/polarizer is a single unit, which advantageously reduces cost and simplifies operation. A spectograph detects the intensity of the spectral components at different polarity orientations. Because the normal incidence reflectometer, in accordance with the present invention, uses normally incident radiation and an analyzer that rotates relative to the diffracting structure, or vice-versa, the orientation of the grating of the diffracting structure does not affect the accuracy of the measurement. Consequently, different types of sample stages, including X, Y, and Z, as well as r-θ type stages may be used. Further, the normal incidence reflectometer advantageously does not require that

the polarization orientation of the incident light be aligned with the grating of the diffraction structure.

One aspect of the present invention is directed towards an apparatus for measuring one or more parameters of a diffracting structure on a sample, the apparatus includes a radiation source that emits broadband radiation, a polarizing element that polarizes the radiation, which is then normally incident on the diffracting structure. At least one of the polarizing element and the diffracting structure are rotatable such that a plurality of polarization orientations of the polarizing element with respect to the diffracting structure may be achieved. The light is reflected off the diffracting structure, passes through the polarizing element and received by a spectrograph that detects the intensity of spectral components of said polarized beam at different polarization orientations of the polarizing element with respect to the diffracting structure. Thus, multiple orientations of the polarization of the reflected light may be received by the spectrograph.

Another aspect of the present invention includes an apparatus for measuring one or more parameters of a diffracting structure on a sample, the apparatus includes a radiation source that emits broadband radiation that is normally incident on the diffracting structure, a polarizing element that is in the beam path of the radiation, an r-θ sample stage that holds the sample with the diffracting structure, and a spectrograph that detects the intensity of spectral components of radiation reflected off said diffracting structure. The polarizing element is positioned such that the radiation passes through the polarizing element toward said sample, the radiation is reflected off the diffracting structure on the sample, the reflected radiation passes through the polarizing element, and the polarizing element is rotatable to produce a relative rotation between said polarizing element and said diffracting structure. The spectrograph detects the intensity of spectral components of the reflected radiation after passing through the polarizing element at a plurality of polarization orientations between the polarizing element and the diffracting structure.

Another aspect of the present invention includes a computer system including a computer coupled to the spectrograph and that receives the spectrograph signals, includes computer instructions for analyzing the spectrograph signals and extracting spectral information from the signals. The computer instructions also include instructions for generating an optical model of the diffracting structure, such as through rigorous coupled-wave analysis, calculating the spectral information from the optical model and curve fitting the optical model to the extracted spectral information, while adjusting variable parameters of the diffracting grating, such as height, pitch, sidewall angle, and critical dimension to achieve a best fit. In one embodiment, the computer

system includes instructions to perform a non-linear multivariate regression process to adjust the parameters of the optical model.

Another aspect of the present invention is directed towards a method of measuring at least one parameter of a diffracting structure, including directing normally incident radiation at a plurality of wavelengths and at a plurality of polarization orientations at the diffracting structure, the radiation reflecting off and diffracted by the diffracting structure on the sample; analyzing the radiation that is reflected off and diffracted by the diffracting structure to produce an output beam with the same polarization orientations; detecting the intensity of spectral components of the output beam at the plurality of polarization orientations; and using the detected intensities of the spectral components of the output beam to determine at least one parameter of the diffracting structure. The method may also include generating a reference database of at least one parameter related to different diffracting structures for a plurality of wavelengths and the plurality of polarity orientations and comparing the detected intensities of the spectral components to the database to determine at least one parameter of said diffracting structure.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 is a schematic diagram of a normal incidence reflectometer with a rotatable analyzer/polarizer that may be used to measure diffracting structures, in accordance with an embodiment of the present invention.

Fig. 2 is a flow chart describing the process of calibrating normal incidence reflectometer.

Fig. 3 is a flow chart showing the process of acquiring sample data in accordance with an embodiment of the present invention.

Fig. 4 is a flow chart of the process of extracting spectral information in accordance with the present invention.

Fig. 5 is a flow chart of the process of data analysis in accordance with the present invention.

DETAILED DESCRIPTION

Fig. 1 is a schematic diagram of a normal incidence reflectometer 100 with a rotatable analyzer/polarizer 122 and that may be used to measure diffracting structures, in accordance with an embodiment of the present invention. The use of a single polarizing element as a rotatable analyzer/polarizer 122, advantageously, permits measurement of diffracting structures with a reduced number of parts. Moreover, normal incidence reflectometer 100 may be used as a

reflectometer to measure non-diffracting structures. Thus, normal incidence reflectometer 100 advantageously need not be a dedicated metrology tool that is used to measure only diffraction gratings, but may be used for other reflectometer-type applications as well.

Normal incidence reflectometer 100 includes a broadband light source 102, such as a UV-visible light source with wavelengths, e.g., between 200nm to 800nm, that produces unpolarized light. The unpolarized light is collected and collimated by lens 104. Beam splitter 106 directs a portion of the collimated, broadband, unpolarized light beam toward the sample that is held on a movable sample stage 118. The sample may be, e.g., a diffraction grating structure 114 on a patterned silicon wafer 116. It should be understood, of course, that grating structure 114 is typically very small and that its size shown in Fig. 1 is exaggerated for the sake of clarity.

Disposed between the beam splitter 106 and the sample 114 is the rotatable analyzer/polarizer ("RAP") 122. The light reflected by beam splitter 106 toward the sample passes through the RAP 122 and is linearly polarized. The rotation of RAP 122 is controlled by a computer 136 in a manner known to those skilled in the art. In another embodiment, RAP 122 is stationary while computer 136 rotates sample stage 118 so that the grating structure 114 is rotated relative to RAP 122.

The RAP 122 passes only the electric field component of the light that is coincident with the polarization axis of the RAP 122 and thus controls the orientation of the light that is incident on the sample. The RAP 122 may be, e.g., Glan Taylor air-spaced polarizer, a dichroic Poloroid sheet, or any other appropriate linearly polarizing device. The light from RAP 122 is focused by objective 108 so that the light is normally incident on grating structure 114. While marginal rays 110 and 112 are at small angles from the normal ray 120 on the sample, the angles are too small to see any polarization effects that occur in conventional ellipsometers. Because RAP 122 is rotated relative to the diffraction structure 114, i.e., RAP 122 and/or diffraction structure 114 is rotated, the polarization orientation of the incident light need not be aligned with the grating of the diffraction structure 114 prior to the metrology process. Consequently, normal incidence reflectometer 100 may be used, advantageously, with a wafer stage 118 that is capable of any or all of x, y, z, and/or Θ movement, as well as a stage that is capable of r-θ movement only.

Diffracted light from the grating structure 114 is re-collimated by lens 108 and passes through the RAP 122, which linearly polarizes the light. The light has an electric field component that is either parallel (sometimes called TE or S-polarization) or perpendicular (sometimes called TM or P-polarization) to the lines of the grating structure 114. The light that

is diffracted from grating structure 114 will have a different electric field component intensities and phase than the light that is incident on the structure 114. The RAP 122 passes only the electric field component of the reflected beam that is coincident with the polarization axis of the RAP 122. Thus, RAP 122 advantageously permits detection of different spectral components of the diffracted light.

The light then passes through the beamsplitter 106. The light is then focused by lens 124 to the entrance slit of a spectrograph 126. In an another embodiment, lens 108 may be replaced with a microscope objective and lens 124 removed. Spectrograph 126 may be a conventional CCD, PDA, or similar type spectrograph that disperses the full spectrum of the polarized light into spectral components across an array of detector pixels. Each pixel corresponds to a different wavelength, and thus the spectrograph 126 generates a spectrograph signal, $S(\lambda)$, as a function of wavelength λ that is transmitted to computer 136. The signal $S(\lambda)$ is corrected for electronic background as is well known in the art. Because the RAP 122 is rotated through a discrete set or continuous set of angles, Θ, from 0 to 360 degrees, the signal $S(\lambda)$ is also a function of angle, $S(\lambda, \Theta)$.

The sample may be viewed and aligned using, e.g., a lamp 130 that produces visible light to provide flood illumination via movable mirror 132. This flood illumination is reflected off mirror 128 to a camera and pattern recognition system 134, which may be coupled to computer 136. The pattern recognition system 134 can provide a measure of orientation of grating structure 114 relative to the RAP 122, if desired, as well as serve as a conventional detector for the sample height. The pattern recognition system 134 provides data to the computer 136, which accordingly adjusts the height of stage 118.

The normal incidence reflectometer 100, in accordance with the present invention, operates in a manner similar to a reflectometer but includes the RAP 122 and uses a relative rotation of the sample, i.e., grating structure 114, and the RAP 122; either RAP 122, sample support 118 or both are rotated. Because components of the normal incidence reflectometer 100, such as beamsplitter 106 and spectrograph 126, have polarization dependent efficiencies, multiple calibrations are performed so that a plurality of orientations of the RAP 122 with respect to the diffraction grating structure 114 are measured relative to some arbitrary machine fiducial. Conventional reflectometers, on the other hand, require only a single calibration and do not use polarizer/analyzer.

Fig. 2 is a flow chart describing the process of calibrating normal incidence reflectometer 100. It should be understood that the calibration process does not need to be performed for every

measurement, but only periodically, e.g., whenever the alignments of the optical elements have changed. The calibration process includes removing the sample from the beam path so that only light reflected from optical elements reaches spectrograph 126 (step 200). The RAP 122 is stepped over a discrete (or continuous) set of angles e.g., from 0 to 360 degrees or 0 to 180 degrees (step 202). A raw spectrograph scan $S_B(\lambda, \Theta)$, for the back reflectance, is acquired at each position, Θ, of the RAP 122 over the set of angles from 0 to 360 degrees (step 204). The back reflectance scan is used to correct for internal reflections. An integral part of any spectrograph scan is the subtraction of dark counts, i.e., measure with light from the source blocked, to measure and correct for electronic background noise, which is well understood in the art.

A non-polarizing (at normal incidence) reference sample, e.g., bare silicon with a native oxide, is placed on the sample stage and the stage height is adjusted, e.g., using the pattern recognition system 134 (step 206). The RAP 122 is stepped over a discrete (or continuous) set of angles from 0 to 360 degrees (step 208) while a raw scan $S_O(\lambda, \Theta)$ from the reference sample is acquired at each position, Θ, of the RAP 122 (step 210).

Thus, the calibration of normal incidence reflectometer 100 produces the function $S_o(\lambda, \Theta)$. Ideally, the calibrations would be performed for continuous orientations of the RAP 122 with respect to the diffraction grating structure 114, but in practice, this may be done at a discrete set of equally spaced angles, e.g., 1 to 5 degrees apart. The function $S_o(\lambda, \Theta)$ for an angle between two of the equally spaced angles would be calculated by a suitable interpolation scheme, e.g., cubic spline, on a wavelength by wavelength basis.

With the normal incidence reflectometer 100 calibrated, the sample data may be acquired. Fig. 3 is a flow chart showing the process of acquiring sample data in accordance with an embodiment of the present invention. The polarizing sample, e.g., wafer 116 with grating structure 114, is placed on the sample stage 118 and the height of the stage 118 is adjusted to focus using, e.g., the pattern recognition system 134 (step 252). The RAP 122 is stepped over the discrete (or continuous) set of angles from 0 to 360 degrees or, alternatively, the stage 118 is rotated, (step 254) and the raw scan $S_S(\lambda, \Theta)$ of the sample is acquired for each position, Θ, of the RAP 122 (step 256). The sample reflectance $R_S(\lambda, \Theta)$ for each position of the RAP 122 is then calculated as follows:

$$R_S(\lambda,\Theta) = \frac{S_S(\lambda,\Theta) - S_B(\lambda,\Theta)}{S_o(\lambda,\Theta) - S_B(\lambda,\Theta)} \cdot R_o(\lambda) \qquad \text{eq. 1}$$

where $R_O(\lambda)$ is the known reflectance of the non-polarizing (at normal incidence) reference sample, e.g., bare silicon with a native oxide from step 206. The reflectance $R_O(\lambda)$ may be determined by measurement or by consulting a library of known reflectances, or calculation from known thicknesses and optical constants of the reference sample. A method of determining absolute reflectance is described in detail in Re. 34,783, reissued Nov. 8, 1994, which is a reissue of U.S. Pat. No. 5,045,704, issued Sep. 3, 1991 to V. Coates and assigned to Nanometrics, Inc., and which is incorporated herein by reference.

With the sample data acquired, the spectral information must be extracted. To do this, it is necessary to analyze the optical system. In the Jones matrix formalism, the electric fields of a plane propagating electromagnetic wave are expressed as a complex valued 2x1 matrix (vector). The effects of polarization altering devices (e.g. beam splitters, diffraction structures, polarizers, etc.) are expressed as 2x2 complex valued transformation vectors. The electric field of the wave exiting the beam splitter 106 towards the spectrograph 126 is given by,

$$\begin{aligned} F(\phi,\Theta) = & \begin{pmatrix} t_S & 0 \\ 0 & t_P \end{pmatrix} \cdot R(-\Theta) \cdot \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} \cdot R(\Theta) \cdot \\ & R(-\phi) \cdot \begin{pmatrix} r_{TM} & 0 \\ 0 & r_{TE} \end{pmatrix} \cdot R(\phi) \cdot \\ & R(-\Theta) \cdot \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} \cdot R(\Theta) \begin{pmatrix} r_S & 0 \\ 0 & r_P \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} \end{aligned} \qquad \text{eq. 2}$$

where, r_{TM} and r_{TE} are the complex valued reflectivities for light polarized perpendicular and parallel to the lines of the diffraction structure, respectively, and, r_s, r_p , and t_s, t_p are the reflectivity coefficients and transmissivity coefficients, respectively, for the s-polarized or p-polarized states of the electric field vector at the beam splitter. The matrix

$$R(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \qquad \text{eq. 3}$$

is a coordinate rotation by some angle, φ, and the matrix

$$\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{eq. 4}$$

corresponds to the polarizing element of the RAP 122. Simplifying the above equation yields

$$F(\phi,\Theta) = A^2\beta(\Theta)\cdot\left[r_{TM}\cdot\cos^2(\phi-\Theta)+r_{TE}\cdot\sin^2(\phi-\Theta)\right]\cdot\begin{pmatrix} t_S\cdot\cos\Theta \\ -t_P\cdot\sin\Theta \end{pmatrix} \qquad \text{eq. 5}$$

where $\beta(\Theta) = r_S a\cdot\cos\Theta + r_P b\cdot\sin\Theta$.

The measurable intensity will then be proportional to

$$\begin{aligned}|F(\phi,\Theta)|^2 &= A^4|\beta(\Theta)|^2\cdot\left(|t_S\cos\Theta|^2+|t_P\sin\Theta|^2\right) \\ &\left[|r_{TM}|^2\cos^4(\phi-\Theta)+|r_{TE}|^2\sin^4(\phi-\Theta)+(r_{TM}r_{TE}^*+r_{TM}^*r_{TE})\cos^2(\phi-\Theta)\sin^2(\phi-\Theta)\right]\end{aligned} \qquad \text{eq. 6}$$

Writing the reflectivities, r_{TM} and r_{TE} in terms of their amplitudes and phases, the cross term in the above equation becomes $(r_{TM}r_{TE}^*+r_{TM}^*r_{TE}) = 2\cdot|r_{TM}|\cdot|r_{TE}|\cdot\cos\Delta$ where $\Delta = \varphi_{TE}-\varphi_{TM}$ is the phase difference between TE and TM reflectivities. In the special case when, $r_{TM} = r_{TE} = r_O$, equation 6 simplifies to

$$|F_O(\phi,\Theta)|^2 = A^4|\beta(\Theta)|^2\cdot\left(|t_S\cos\Theta|^2+|t_P\sin\Theta|^2\right)\cdot|r_O|^2 \qquad \text{eq. 7}$$

Now we have the following relationship where to the left of the equality sign we have known or measurable quantities and on the right side of the equation are the unknowns to be determined.

$$\begin{aligned}\frac{|F(\phi,\Theta)|^2}{|F_O(\phi,\Theta)|^2}|r_O|^2 &= |r_{TM}|^2\cos^4(\phi-\Theta)+|r_{TE}|^2\sin^4(\phi-\Theta) \\ &+2\cdot|r_{TM}|\cdot|r_{TE}|\cdot\cos\Delta\cdot\cos^2(\phi-\Theta)\sin^2(\phi-\Theta)\end{aligned} \qquad \text{eq. 8}$$

The quantity on the left side is the absolute reflectance of the sample, $R_S(\lambda, \Theta)$, as a function of wavelength λ and the angle Θ of RAP 122 relative to the diffraction grating 114. A method of

determining absolute reflectance is described in detail in Re. 34,783, reissued Nov. 8, 1994, which is a reissue of U.S. Pat. No. 5,045,704, issued Sep. 3, 1991 to V. Coates and assigned to Nanometrics, Inc., and which is incorporated herein by reference.

Fig. 4 is a flow chart of the process of extracting spectral information. The spectral information is extracted by curve fitting the function $R_S(\lambda, \Theta)$ for each wavelength, λ, using a non-linear regression analysis, e.g., the Levenberg-Marquardt algorithm, to the following function derived from equation 8.

$$R(\Theta) = A \cdot \cos^4(\phi - \Theta) + B \cdot \sin^4(\phi - \Theta) + C \cdot \cos^2(\phi - \Theta) \cdot \sin^2(\phi - \Theta) \qquad \text{eq. 9}$$

where adjustable parameters, i.e., measurables, are ϕ, A, B, and C, which indicates that the minimum number of RAP 122 orientations needed is four (step 272).

It should be understood that other methods of spectral information extraction may be used, for example, equation 2 may be inverted and the parameters directly calculated. This is advantageous because no iteration is required, but may have somewhat limited application, e.g., may not provide an accurate answer for all functions. In particular, data can be acquired at four equally spaced angles δ, $\delta + \pi/4$, $\delta + \pi/2$, and $\delta + 3\pi/4$ over one 180 degree period where $\delta = \phi - \Theta_1$ and Θ_1 is the first RAP 122 angle of acquisition. Make the substitutions

$$x = \cos^2(\phi - \Theta); \qquad \alpha = A + B - C; \qquad \beta = C - 2B; \quad \gamma = B \qquad \text{eq. 10}$$

into equation 9 to obtain the following system of four equations.

$$R_{S1} = \alpha \cdot x_1^2 + \beta \cdot x_1 + \gamma; \qquad \text{eq. 11}$$

$$R_{S2} = \alpha \cdot x_2^2 + \beta \cdot x_2 + \gamma; \qquad \text{eq. 12}$$

$$R_{S3} = \alpha \cdot x_3^2 + \beta \cdot x_3 + \gamma; \text{ and} \qquad \text{eq. 13}$$

$$R_{S4} = \alpha \cdot x_4^2 + \beta \cdot x_4 + \gamma. \qquad \text{eq. 14}$$

Note x_1, x_2, x_3, x_4 are all functions of δ so the four unknowns are α, β, γ, and δ. The above system can be inverted according to the following equations.

$$\delta = \arctan\left[\frac{R_{S2} - R_{S4}}{R_{S3} - R_{S1}}\right]; \qquad \text{eq. 15}$$

$$\alpha = 2 \cdot \left[\frac{R_{S1} + R_{S3} - R_{S2} - R_{S4}}{\cos(4\delta)}\right]; \qquad \text{eq. 16}$$

$$\beta = \sqrt{(R_{S1} - R_{S3})^2 + (R_{S2} - R_{S4})^2} - \alpha \text{ ; and} \qquad \text{eq. 17}$$

$$\gamma = \frac{1}{4} \cdot (R_{S1} + R_{S2} + R_{S3} + R_{S4} - \frac{3\alpha}{2} + 2\beta). \qquad \text{eq. 18}$$

Finally, A, B, and C may be calculated according to:

$$A = \alpha + \beta + \gamma; \qquad B = \gamma; \qquad C = \beta + 2\gamma. \qquad \text{eq. 19}$$

As indicated in Fig. 4, the R_{TE}, R_{TM} and cosΔ are then calculated (step 274), as follows:

$$R_{TE}=A;\ R_{TM}=B;\ \cos\Delta = \frac{C}{2\sqrt{AB}};\ \text{or} \qquad \text{eq. 20}$$

$$R_{TE}=B;\ R_{TM}=A;\ \cos\Delta = \frac{C}{2\sqrt{AB}}. \qquad \text{eq. 21}$$

Because of the symmetry of equation 2, it is not known which equation of equations 20 and 21 is correct. The correct equation is determined using knowledge of the orientation of the diffracting structure taken from the manufacturing process and knowledge of the approximate orientation of the RAP 122, e.g., as determined by pattern recognition system 134. The TM and TE orientations are always 90 degrees apart, and thus, the polarization angle of the RAP 122 does not need to be known with great accuracy, ±20 degrees should be adequate. There are two analyzer angles, Θ_{TE} and $\Theta_{TE} + \pi$ when the analyzer will pass only the TE component and two analyzer angles, $\Theta_{TE} \pm \pi/2$ when the analyzer will pass only the TM component. Because the electric field of the reflected beam can be written as a superposition of TE and TM components relative to the diffraction grating, the reflected intensity, $R_S(\lambda)$, will have oscillatory variation

with Θ reaching extrema at Θ_{TE}, $\Theta_{TE} + \pi/2$. The absolute reflectances for TE and TM components are labeled $R_{TE}(\lambda)$ and $R_{TM}(\lambda)$, respectively. Whether a particular extrema corresponds to TE or TM light can be determined from the knowledge of the sample orientation and the pattern recognition system. The approximate orientation of any polarizing device can be measured or approximated by anyone skilled in the art.

Actual measurements can be made in either an absolute fashion where the RAP 122 is driven to the TM and TE positions by computer 136 or in a relative fashion where the analyzer is rotated continuously.

Another method that can be used to extract spectral information is performed by, first, loading the wafer on the sample stage with the diffraction structure lines approximately parallel to the RAP 122 transmission axis. Then, measure $R_S(\Theta)$ for a plurality of values of Θ, e.g., 5 to 20 values, varying from -20 degrees to +20 degrees. Plot $R_S(\Theta)$ and fit this function to a parabola, identifying the extremum as Θ_{TE}. Rotate the RAP 122 to $\Theta=\Theta_{TE}$, and measure R_S. This would be identified as R_{TE}. Finally, rotate the RAP 122 to $\Theta=\Theta_{TE} \pm \pi/4$ and measure R_S. This would be identified as R_{TM}.

Advantageously, because normal incidence reflectometer 100 includes a rotating element, i.e., the RAP 122 and/or sample stage 118, and operates at normal incidence, the orientation of the grating structure 114 does not affect the accuracy of the measurement. The optics are always aligned to the structure. This is of particular advantage when coupled with an r-θ sample stage.

The reflectances $R_{TE}(\lambda)$ and $R_{TM}(\lambda)$ from the polarizing diffraction grating can be used to deduce information about the grating such as pitch, linewidth, and lineshape via exact modeling of $R_{TE}(\lambda)$, $R_{TM}(\lambda)$, and $\cos\Delta(\lambda)$ spectra using, e.g., rigorous coupled wave analysis ("RCWA"). For more information regarding RCWA, see M. G. Moharam and T. K. Gaylord, "Rigorous coupled-wave analysis of planar grating diffraction", J. Opt. Soc. Am., Vol. 71, No. 7, pp. 811-818, (1983); M. Moharam et al., "Stable implementation of the rigorous coupled wave analysis for surface-relief gratings: enhanced transmittance matrix approach," J. Opt. Soc. Am. A., Vol. 12, No. 5, pp. 1077-1086 (1995); T. Gaylord et al., "Analysis and Applications of Optical Diffraction by Gratings," Proceedings of the IEEE, Vol. 73, No. 5, pp. 894-937 (1985), N. Chateau and J.P. Hugonin, " Algorithm for the rigorous coupled-wave analysis of grating diffraction," J. Opt. Soc. Am. A, Vol. 11, No. 4, April 1994, pp. 1321-1331; and M.G. Gaylord et. al., "Formulation for stable and efficient implementation of the rigorous coupled-wave

analysis of binary grating," J. Opt. Soc. Am. A, Vol. 12, No. 5, May 1995, pp. 1068-1076, which are incorporated herein by reference.

A difficulty with RCWA analysis has been the very large amount of computation that must be done to accurately simulate the optical response of a grating structure. In particular, the reflected TM light calculation converges very slowly. Most solutions have been to build large libraries of response curves offline and search the library for a best match at the time of measurement. The present invention, advantageously, allows for the separation of the TE and TM components. A library can be searched, matching both TE and TM components for a rough estimation of the diffracting structure and then relatively fast, real time iteration on normal incidence TE light can be used to refine the measurement. The Levenberg-Marquardt non-linear multivariate regression process is used to adjust the parameters in the RCWA model such that the reflectance spectrum predicted by the model matches a given measured spectrum as closely as possible. The Levenberg-Marquardt non-linear multivariate regression is discussed in "Numerical Recipes: The Art of Scientific Computing," by W. Press, et al., Cambridge University Press, 1986, Section 14.4, pp. 521-528.

Fig. 5 is a flow chart of the process of data analysis in accordance with the present invention. The data analysis may be performed, e.g., by computer 136, which executes a computer program with appropriate computer instructions. The spectral data, i.e., $R_{TM}(\lambda)$, $R_{TE}(\lambda)$, and $\cos\Delta$, is acquired as discussed above in reference to Figs. 2, 3, and 4 (step 302). An optical model is constructed to simulate the structure on the sample under test and the spectral data is calculated (step 304). The optical model is constructed using, e.g., the RCWA model, with variable parameters, such as layer thickness, grating linewidth, sidewall angle of the grating, and optical constants of the materials in the model.

Computer 136, or another computer that is in communication with computer 136, executes a computer program with computer instructions to calculate the model spectrum using the RCWA model as described by the following pseudo-code. Calculations of the model spectrum are performed for each wavelength. Inputs to the calculation are the optical constants and thickness of each layer in the model, and all grating parameters for any grating layer in the model. Note that "I" designates the identity matrix, and that all matrices and vectors referred to below are defined in Moharam, Pommet, Grann, and Gaylord, J. Opt. Soc. Am. A, vol. 12, No. 5, 5/1995, pp. 1077-1086, which is incorporated herein by reference. Unless otherwise noted all matrices are of dimension N by N, where N=2*number of diffracted orders + 1.

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Beginning:
    Calculate initial matrix f (equal to the identity matrix);
    Calculate initial matrix g (function of substrate parameters only);

    Loop over layers in the model, starting at the bottom layer (next to substrate);

        Calculate matrix E of Fourier coefficients for the dielectric function;
        Calculate matrix P of Fourier coefficients for the inverse of the dielectric
            function;
        Invert E and store in Einv;
        Invert P and store in Pinv;
        Calculate x-component of the wavevector for each diffracted order, place
            on diagonal of the diagonal matrix Kx;
        Construct eigenproblem matrix from the above three results:
            If TE mode, eigenproblem matrix is:
                A=Kx*Kx-I;
            Else if TM mode, eigenproblem matrix is:
                A=Pinv*(Kx*Einv*Kx – I)
            End if
        Solve for eigenvalues and eigenvectors of matrix A;
        Store eigenvalues on diagonal of (diagonal) matrix Q.
        Store eigenvectors in columns of matrix W;
        If TE mode;
            Calculate matrix V=W*Q;
        Else if TM mode;
            Calculate matrix V=P*W*Q;
        End if
        Calculate diagonal matrix X – diagonal elements are exp(-Qii*thickness)

        Construct temporary 2N*2N matrix as follows:
            Upper left block is –W;
            Upper right block is f;
            Lower left block is V;
```

Lower right block is g;

Invert this temporary matrix;

Let Temp00 be the upper left block of the inverted temporary matrix;

Let Temp01 be the upper right block of the inverted temporary matrix;

Calculate matrix a=Temp00*W*X+Temp01*V*X;

Calculate new f matrix as f=W*(I+X*a);

Calculate new g matrix as g=V*(I-X*a);

Repeat for Next Layer

Comment: Construct and solve final system of linear equations to get Reflected fields for each diffracted order;

Calculate diagonal matrix ZI, with diagonal elements equal to the z component of the wavevector of each diffracted order in the ambient.

Calculate the Coefficient matrix alpha=$g*f^{-1}+j*ZI$;

Construct vector beta, where

If I= # of harmonics

Beta[I]=j-$(g*f^{-1})_{I,I}$

Else

Beta[I]=$(g*f^{-1})_{I,NumHarmonics}$

End if

Solve system of linear equations defined by alpha and beta;

Solution of this system yields the complex amplitudes of the reflected orders;

Calculate the reflectance of the zeroth diffracted order as the square of the Magnitude of the complex amplitude of the zeroth reflected order;

End;

As shown in Fig. 5, once the data from the optical model is calculated, the match between the measured data and the calculated data is evaluated (step 306). The evaluation of the match

may be performed using the Mean-Squared Error (MSE) between the measured and calculated data. If the measured data points are denoted as $y_m(\lambda_I)$ and the calculated data points are denoted as $y_c(\lambda_I)$, then the MSE is given by:

$$MSE = \sum \frac{(y_m(\lambda_I) - y_c(\lambda_I))^2}{N - M} \quad \text{eq. 22}$$

Where N is the total number of data points and M is the total number of variable parameters in the model. Note that if the measured and calculated data are identical, the MSE value is zero and that the smaller the value of MSE the better the match between the measured and calculated data.

Assuming the MSE value is not zero, the values of the variable parameters in the optical model are appropriately adjusted (step 308), for example, using the Levenberg-Marquardt algorithm, and the optical data is recalculated using the optical model and the adjusted parameter values (step 310). The match between the measured and calculated data is then reevaluated (step 312) to see if the new MSE is less than the previous value. If so, the new parameter values have improved the fit between the measured and calculated data. A decision is made whether a best fit has been derived (step 314), which is determined when adjusting the values in the model does not reduce the value of the MSE any further. Thus, if a best fit has not been achieved, i.e., the fit is still improving (or is worse), the process goes back to step 308, where the values of the variable parameters are appropriately adjusted. If the best fit is achieved, then the variable parameters are reported as the measurement result (step 316).

Computer 136, or another computer that is in communication with computer 136, executes a computer program with computer instructions to perform the process of Fig. 5, as described by the following pseudo-code. It should be understood, that part of the process of Fig. 5 includes the calculation of the model spectrum using the RCWA model, discussed above.

```
Load measured spectrum into Rmeas();
Load measured wavelengths into Wvls();

Set initial values of all model parameters;
Set initial value of Marquardt parameter alpha=0.001;

Calculate initial spectrum from the model, store in Rcalc();
```

Calculate initial MSE value;

Beginning of Main Loop:

For each variable parameter in the model:

Add small increment to the variable parameter;

Recalculate the spectrum from the model with the incremented parameter;

Calculate array of derivatives of MSE with respect to the variable parameter from Newton's approximation at each wavelength – $df/dx= (f(x+\delta)-f(x))/\delta$;

Restore variable parameter to its original value;

End of loop on variable parameters;

Calculate Hessian matrix from calculated derivative arrays and the Marquardt parameter;

Calculate Gradient vector from calculated derivative arrays;

Solve system of linear equations defined by Hessian matrix and Gradient vector;

Add solution to the vector of variable parameters;

Recalculate the spectrum from the model using these new parameter values;

Calculate the MSE for this new spectrum;

If the new MSE is less than the previous MSE, retain these values, divide the Marquardt parameter by 10, and go back to the beginning of the main loop and repeat. If convergence criteria have been reached go to the end. Convergence criteria are change in MSE less than some small value (10^{-10}, for example) or the maximum number of iterations has been reached.

Else the new MSE is larger than the previous MSE;

Restore variable parameter values back to what they were at the beginning of the iteration.

Multiply the Marquardt parameter by 10;

If the maximum number of iterations is exceeded, go to the end.

Go to the beginning of the main loop for the next iteration.

End if;

End of Main Loop;

End:

Although the invention has been described with reference to particular embodiments, the description is only an example of the invention's application and should not be taken as a limitation. In particular, although the above description is directed mostly to a system that uses a RCWA analysis coupled with real-time non-linear regression analysis, e.g., the Levenberg-Marquardt analysis, to measuring a diffraction grating structure, other methods of analysis may be used if desired, such as RCWA analysis, an initial reference database search followed by real-time non-linear regression analysis, e.g., the Levenberg-Marquardt analysis. Various other adaptations and combinations of features of the embodiments disclosed are within the scope of the invention as defined by the following claims.